

CONF - 820304 - -11

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

LA-UR--82-3572

DDO 004705

MASTER

TITLE: REVIEW OF SOLUTION APPROACH, METHODS, AND
RECENT RESULTS OF THE TRAC-PF1 SYSTEM CODE

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SUBMITTED TO: 1983 Mathematics and Computation Topical Meeting
American Nuclear Society
March 28-31, 1983
Salt Lake City, Utah

Approved for Release by NSA on 09-11-2013 pursuant to E.O. 13526

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REVIEW OF SOLUTION APPROACH, METHODS, AND
RECENT RESULTS OF THE TRAC-PF1 SYSTEM CODE

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The current version of the Transient Reactor Analysis Code (TRAC-PF1) was created to improve on the capabilities of its predecessor (TRAC-PD2) for analyzing slow reactor transients such as small-break loss-of-coolant accidents. TRAC-PF1 continues to use a semi-implicit finite-difference method for modeling three-dimensional flows in the reactor vessel. However, it contains a new stability-enhancing two-step (SETS) finite-difference technique for one-dimensional flow calculations. This method is not restricted by a material Courant stability condition, allowing much larger time-step sizes during slow transients than would a semi-implicit method. These have been successfully applied to the analysis of a variety of experiments and hypothetical plant transients covering a full range of two phase flow regimes.

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REVIEW OF SOLUTION APPROACH, METHODS, AND RECENT RESULTS OF THE TRAC-PF1 SYSTEM CODE

INTRODUCTION

In this paper we provide a simple description of the numerical methods used to model two-phase flow in version PF1 of the Transient Reactor Analysis Code (TRAC-PF1)¹ and summarize recent results produced by this code. The main difference in methods between this and previous versions of TRAC² is in one-dimensional modeling of flow. It is now possible to model an entire reactor system with one-dimensional components. This allows the user to take advantage of the new stability-enhancing two-step method (SETS),^{3,4} which removes the material Courant stability limit from all one-dimensional regions. With this approach, it is possible to model many problems with much larger time steps than were previously possible. If needed, a three-dimensional vessel option is available. However, this option still uses a semi-implicit finite-difference technique, and is therefore restricted by the material Courant limit.

The SETS method was designed to propagate information needed for stability with minimal implicit coupling between spatial nodes. Information about pressure-wave propagation is provided with a basic step, which is simply a semi-implicit equation set. A stabilizing step then is added to provide information about the transport of fluid density, energy, and momentum across cell boundaries. Because the stabilizing step is separated from the basic step, this approach has the further advantage that existing semi-implicit codes can be converted to the SETS method with relative ease.

BASIC EQUATIONS

To demonstrate the TRAC-PF1 numerical methods, we will consider a simplified model for one-dimensional, single-phase flow in a pipe. The differential equations for this model are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho V = 0 \quad , \quad (1)$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \rho e V = -p \nabla \cdot V + h (T_w - T) \quad , \quad (2)$$

and

$$\frac{\partial V}{\partial t} + \nabla \cdot V V = -\frac{1}{\rho} \nabla p - K V |V| \quad . \quad (3)$$

Here, K is a wall friction coefficient that may be a function of velocity and fluid properties, h is a heat-transfer coefficient multiplied by the heat-transfer area per volume of fluid, and T_w is a pipe wall temperature.

A staggered spatial mesh was used for the finite-difference equations, with thermodynamic properties evaluated at the cell centers and the velocity evaluated at the cell edges. Only difference equations on the one-dimensional version of this mesh will be demonstrated, but the generalization to two- and three-dimensional versions is not difficult. To ensure stability and to maintain consistency with differencing in previous TRAC versions, flux terms at cell edges use donor cell averages of the form

$$\langle YV \rangle_{j+1/2} = \begin{cases} Y_j V_{j+1/2} & , \quad V_{j+1/2} \geq 0 \\ Y_{j+1} V_{j+1/2} & , \quad V_{j+1/2} < 0 \end{cases} \quad . \quad (4)$$

Here Y may be any state variable. Other forms of this average may maintain stability with higher order spatial accuracy but they have not been carefully studied. With this notation, the one-dimensional finite-difference divergence operator is

$$\nabla_j \cdot (YV) = (A_{j+1/2} \langle YV \rangle_{j+1/2} - A_{j-1/2} \langle YV \rangle_{j-1/2}) / \text{vol}_j, \quad (5)$$

where A is the area of the cell edge and vol_j the cell volume. The term $\nabla \cdot YV$ becomes

$$\nabla_{j+1/2} v_{j+1/2} = \begin{cases} v_{j+1/2} (v_{j+1/2} - v_{j-1/2}) / \Delta x_{j+1/2}, & v_{j+1/2} \geq 0 \\ v_{j+1/2} (v_{j+3/2} - v_{j+1/2}) / \Delta x_{j+1/2}, & v_{j+1/2} < 0 \end{cases}, \quad (6)$$

where $\Delta x_{j+1/2} = 0.5 (\Delta x_j + \Delta x_{j+1})$. This choice of $\Delta x_{j+1/2}$ for equation 6 was necessary for more accurate calculation of pressure drops in pipes modeled with a nonuniform mesh than is provided with a donor cell, $\Delta x_{j+1/2}$.

For the flow model given by equations 1-3, the combination of basic and stabilizer equation sets can be written in several ways without significantly affecting the results. For example, the stabilizer step may precede the basic step for all equations, or the basic step may be done before the stabilizer step. When the SETS method is adapted to the two-fluid model for two-phase flow, several orderings of the difference equations can cause growing oscillations from feedback through interfacial friction terms. Some of these feedback problems are rather subtle and only occur when the one-dimensional mesh forms a closed loop. One ordering, that is always stable begins with the stabilizer step for the equations of motion, is followed by a solution of the basic equation set for all equations, and ends with a stabilizer step for the mass and energy equations. For this ordering, the SETS finite-difference equations for equations 1-3 are:

STABILIZER EQUATION OF MOTION

$$\begin{aligned}
 & (\tilde{v}_{j+1/2}^{n+1} - v_{j+1/2}^n) / \Delta t + v_{j+1/2}^n v_{j+1/2} \tilde{v}^{n+1} \\
 & + \beta (\tilde{v}_{j+1/2}^{n+1} - v_{j+1/2}^n) v_{j+1/2} \tilde{v}^n \\
 & + \frac{1}{\langle \rho \rangle_{j+1/2}^n \Delta x_{j+1/2}} (p_{j+1}^n - p_j^n) \\
 & + \kappa_{j+1/2}^n (2 \tilde{v}_{j+1/2}^{n+1} - v_{j+1/2}^n) |v_{j+1/2}^n| = 0 \quad ,
 \end{aligned} \tag{7}$$

where

$$\beta = \begin{cases} 0, & v_{j+1/2} \tilde{v}^n < 0 \\ 1, & v_{j+1/2} \tilde{v}^n > 0 \end{cases} ;$$

BASIC EQUATIONS

$$\begin{aligned}
 & (v_{j+1/2}^{n+1} - v_{j+1/2}^n) / \Delta t + v_{j+1/2}^n v_{j+1/2} \tilde{v}^{n+1} \\
 & + \beta (v_{j+1/2}^{n+1} - v_{j+1/2}^n) v_{j+1/2} \tilde{v}^n + \frac{1}{\langle \rho \rangle_{j+1/2}^n \Delta x_{j+1/2}} (\tilde{p}_{j+1}^{n+1} - \tilde{p}_j^{n+1}) \\
 & + \kappa_{j+1/2}^n (2 v_{j+1/2}^{n+1} - v_{j+1/2}^n) |v_{j+1/2}^n| = 0 \quad ;
 \end{aligned} \tag{8}$$

$$(\tilde{p}_j^{n+1} - p_j^n) / \Delta t + v_j \cdot (\rho^n v^{n+1}) = 0 \quad ; \tag{9}$$

$$\begin{aligned}
 & (\tilde{p}_j^{n+1} \tilde{e}_j^{n+1} - p_j^n e_j^n) / \Delta t + v_j \cdot (\rho^n e^n v^{n+1}) \\
 & + \tilde{p}_j^{n+1} v_j \cdot (v^{n+1}) - h_j^n (T_{\omega j}^n - T_j^{n+1}) = 0 \quad ;
 \end{aligned} \tag{10}$$

and

STABILIZER MASS AND ENERGY EQUATIONS

$$(\rho_j^{n+1} - \rho_j^n) / \Delta t + \nabla_j \cdot (\rho^{n+1} v^{n+1}) = 0 \quad ; \quad (11)$$

$$\begin{aligned} (\rho_j^{n+1} e_j^{n+1} - \rho_j^n e_j^n) / \Delta t + \nabla_j \cdot (\rho^{n+1} e^{n+1} v^{n+1}) \\ + \tilde{p}_j^{n+1} \nabla_j \cdot (v^{n+1}) - \bar{h}_j^n (T_{w,j}^n - \tilde{T}_j^{n+1}) = 0 \quad . \end{aligned} \quad (12)$$

A tilde above a variable indicates that it is the result of an intermediate step and is not the final value for the time step.

Equations 8-10 are very similar to a one-dimensional single-phase version of the difference equations used for the TRAC vessel component. These semi-implicit equations can be obtained by dropping all tildes from equations 8-10 and replacing the VV in equation 8 with $V_{j+1/2}^n \nabla_{j+1/2} v^n$. In addition, the pressure work term for the three-dimensional energy equation is $p^n \nabla \cdot v^{n+1}$ rather than $p^{n+1} \nabla \cdot v^{n+1}$. This change in the work term was made because in the three-dimensional numerics, only the linearized flow equations are solved, and the linearized form of $p^{n+1} \nabla \cdot v^{n+1}$ can produce nonphysical results for sudden, unexpected changes in pressure.

The heat-transfer term $\bar{h}^n (T_w^n - T^{n+1})$ was written in this form to minimize coupling between the hydrodynamic and heat-transfer solution procedures. To maintain stability in regions of rapid change of h , \bar{h}^n is an average of the heat-transfer coefficient evaluated at time level n and the averaged coefficient from level $n-1$ ($\bar{h}^n = 0.45 h^n + 0.55 \bar{h}^{n-1}$). An experimental version of TRAC-PF1 exists with fully implicit heat-transfer terms, $[h^{n+1} (T_w^{n+1} - T^{n+1})]^{.5}$.

The material Courant stability limit is eliminated by treatment of the terms VV , $V \cdot \rho V$, and $V \cdot \rho e V$ during the two steps. These are the terms involved in the information propagation that was discussed in the Introduction. Protection against some other instabilities has been obtained with the particular form for the friction terms and the use of nonzero values of β in the VV terms. These special terms for friction and VV are obtained by linearizing similar terms that are fully implicit in velocity ($K_{j+1/2}^n \frac{v_{j+1/2}^{n+1}}{|v_{j+1/2}^{n+1}|}$ and $\frac{v_{j+1/2}^{n+1}}{|v_{j+1/2}^{n+1}|} \nabla_{j+1/2} v^{n+1}$).

Equation 7 simply represents a tridiagonal linear system in the unknown \tilde{v}^{n+1} and is solved first. Next, the coupled nonlinear system given by equations 8-10 is solved. Details of the solution procedure for these equations are presented in the following section. Once these equations are solved, \tilde{v}^{n+1} is known; hence equations 11 and 12 are simple tridiagonal linear systems, with unknowns ρ_j^{n+1} and $\rho_j^{n+1} e_j^{n+1}$, respectively.

When this equation set is adapted to flow in complex piping networks, the pure tridiagonal structure is lost. However, the matrices are still sparse and easily solved.

A standard linear stability analysis predicts unconditional stability for this set of difference equations; a result verified by a large number of computational test problems. However, at very large time steps, functional forms for the friction factor containing a strong velocity dependence can drive instabilities, as can a strong void-fraction dependence for interfacial friction in the two-fluid model. This is why the method is referred to as stability enhancing rather than unconditionally stable.

Because the basic form of the finite-difference operators (both spatial and temporal) is consistent between the two steps, the order of accuracy of the full SETS equations is the same (first order in space and time) as the basic semi-implicit equations 8-10. This consistency appears necessary to prevent the development of feedback oscillations between the two steps. It also has the advantage of ensuring that, for modest time-step sizes, the results of any SETS calculation will approach those of the basic semi-implicit equations.

We have found the SETS method particularly valuable when applied to the full two-fluid model of two-phase flow. For this model the stabilizer equations add less than 20% to the computational cost per cell per step of the basic equation set. A fully implicit method multiplies this cost by a factor of 6. The full finite-difference equations for the two-fluid model are given in the TRAC-PF1 manual, including a useful variation on the finite-difference divergence operator.

SOLUTION OF THE BASIC EQUATION SET

The first step in the solution of the basic (semi-implicit) equation set is to rearrange the motion equation to obtain the new time velocity as a linear function of new time pressures. For equation 8 this results in the relation

$$v_i^{n+1} = \frac{v_i^n - \Delta t [v_i^n \cdot \nabla_i (\hat{v}^{n+1} - \beta \hat{v}^n) - K_i^n v_i^n |v_i^n| + \frac{\tilde{p}_{j+1}^{n+1} - \tilde{p}_j^{n+1}}{\langle \rho \rangle_i^n \Delta x_j}]}{1 + \Delta t (2K_i^n |v_i^n| + \beta \nabla_i \hat{v}^n)}, \quad (13)$$

where $\nabla_i = \partial / \partial x_i + 1/2$. Given this relation, the derivatives of velocity with respect to pressure are

$$\frac{dv_{j+1/2}^{n+1}}{dp_j^{n+1}} = \frac{\Delta t}{\langle \rho \rangle_j^n \Delta x_i (1 + K_j^n \Delta t |v_j^n| + \Delta t \beta v_j \tilde{v}^n)} ; \quad (14)$$

and

$$\frac{dv_{j+1/2}^{n+1}}{dp_{j+1}^{n+1}} = - \frac{dv_{j+1/2}^{n+1}}{dp_j^{n+1}} . \quad (15)$$

Equation 13 and thermodynamic equations giving $\rho(p,T)$ and $e(p,T)$ are substituted into equations 9 and 10 to give a coupled system of nonlinear equations with unknowns p_j^{n+1} and T_j^{n+1} (tildes have been dropped to simplify notation). The solution of this system is obtained with a standard Newton iteration. Given the latest guesses $p_j'^{n+1}$ and $T_j'^{n+1}$ for pressures and temperatures, we assume the solution to be

$$p_j^{n+1} = p_j'^{n+1} + \delta p_j \quad (16)$$

and

$$T_j^{n+1} = T_j'^{n+1} + \delta T_j . \quad (17)$$

The normal procedure for starting this linearization is to make an initial guess for the new time pressure and temperature of $p_j'^{n+1} = p_j^n$ and $T_j'^{n+1} = T_j^n$. However, when using SETS, an extra call to the thermodynamic subroutines can be saved by taking $p_j'^{n+1} = \tilde{p}_j^n$ and $T_j'^{n+1} = \tilde{T}_j^n$.

After substituting equations 13-17 into the basic equation set, making the necessary Taylor series expansions, and after discarding nonlinear terms in δp_j and δT_j , the resulting linear mass and energy equations are in the form

$$B_j \begin{pmatrix} \delta p_j \\ \delta T_j \end{pmatrix} = \underline{b}_j + \underline{c}_j(\delta p_{j+1} - \delta p_j) - \underline{d}_j(\delta p_j - \delta p_{j-1}) \quad , \quad (18)$$

where B is a 2×2 matrix. For the one-dimensional numerics, the first step of the solution procedure is to multiply this equation by B^{-1} (accomplished with a linear system solver), yielding

$$-d'_{1,j} \delta p_{j-1} + (1 + d'_{1,j} + c'_{1,j}) \delta p_j - c'_{1,j} \delta p_{j+1} = b'_{1,j} \quad (19)$$

and

$$\delta T_j = b'_{2,j} + c'_{2,j}(\delta p_{j+1} - \delta p_j) - d'_{2,j}(\delta p_j - \delta p_{j-1}) \quad , \quad (20)$$

where $\underline{b}' = B^{-1}\underline{b}$, etc. All coefficients are stored, and then the set of equations represented by 19 is solved for all δp_j . Finally, the known values for pressure variations are substituted into equation 20 to obtain temperature changes, and are used with equations 14 and 15 for updated velocities. Given these changes, the next guesses for new time pressures and temperatures are generated and used to obtain densities and energies. If changes in δT and δp are too large, these guesses are used to return to equations 16 and 17 to relinearize for another iteration for the one-dimensional equations. As previously noted, the three-dimensional flow equations are not relinearized. In this case, time step controls are used to assure the accuracy of a single linearization.

The principal difference in solution procedures between the one-dimensional and three-dimensional equation sets comes in the actual solution of the linearized pressure equation 19. For one dimension, direct-solution techniques always are employed. If too many cells are present in the three-dimensional model, an iterative method is applied. (See reference 1 or 2.)

Currently, the Jacobian for the system is re-evaluated on each iteration. This may not always be necessary, but for steam-water flows with phase change, it is often important for rapid convergence of the iteration.

CODE APPLICATIONS

Because TRAC-PF1 has been available to the public for only one year, most results have come from code assessment calculations. Before the release of the code, we subjected it to developmental assessment. Following the release of the code to outside users, we began the independent assessment. Developmental assessment is concurrent with the final stages of code development, and the final calculations are made with the released code version. Independent assessment uses a fixed code version, and no model changes are allowed in the code. Both types of assessment compare code calculations to data from various experiment facilities. The experiments include separate-effects tests investigating phenomena such as natural circulation, critical flow, and counter-current flow. However, the bulk of the assessment involves comparisons to data from integral tests that simulate all necessary nuclear-reactor systems and that include multiple phenomena important to reactor safety.

We have analyzed tests from the Marviken critical-flow facility, from the Semiscale facility, an electrically-powered simulator, and from the Loss-of-Fluid-Test Facility (LOFT), a nuclear reactor designed to conduct tests.

The Marviken comparisons⁶ demonstrate the capabilities of the new critical-flow model. The analyses⁷ for Semiscale Tests S-07-10D, S-SB-P1, and S-SB-P7 show data comparisons for small-break loss-of-coolant-accident (LOCA) simulations. Test S-07-10D is a small-break LOCA with delayed emergency core cooling (ECC). Tests S-SB-P1 and S-SB-P7 investigate the sensitivity of a small-break LOCA to pump operation. The analyses⁸ for Semiscale Tests S-UT-6 and S-UT-7 investigate the sensitivity of small-break LOCA to upper-head injection of ECC water. The analysis⁹ of Semiscale Test S-06-3 demonstrated the large-break-LOCA capability of the code. LOFT Tests L5-1 and L8-2, intermediate-break LOCAs, have been analyzed;¹⁰ Test L8-2 had delayed ECC and investigated the effect of restarting the pump. The various data comparisons show that the code can calculate the phenomena important to LOCA.

We are beginning to analyze tests that demonstrate the non-LOCA capabilities of the code. These tests simulate operational transients and the failures of various systems. The initial data comparisons¹¹ are for LOFT Test L9-1/L3-3. The initial phase of this test simulated the loss of feedwater to the secondary and included a delayed reactor scram. The second phase of the test included a failure of the power-operated relief valve on the pressurizer. In addition to demonstrating the capabilities of the code, the analyses showed the importance of detailed modeling of all structural masses. We have analyzed one real reactor transient,¹² the loss-of-feedwater transient at the Crystal River power plant. This transient was less severe than the LOFT Test L9-1/L3-3, but included a detailed modeling of the once-through steam generator.

Currently, the assessment process is continuing with the analyses of additional, more varied tests. Also, Los Alamos is using TRAC-PF1 to analyze hypothesized power-plant transients that are important to the question of pressurized thermal shock to the reactor vessels. Finally, we are using the code to perform large-break-LOCA calculations in support of experiments.

The accumulated experience in the application of TRAC-PF1 indicates that the code generally is applicable to a very wide range of thermal-hydraulic transient and phenomena. The data comparisons have indicated the need for improvement in some of the constitutive relations, but the fundamental set of field equations, together with the differencing scheme and numerical techniques, is very flexible and stable.

CONCLUSIONS

The methods presented here have proven to be extremely reliable tools for reactor safety analysis. They can handle a wide range of fluid conditions and time scales with minimal failures, while maintaining time-step sizes well above those possible with most other techniques. This robustness is due not only to the finite-difference equations themselves, but also to the choice of solution technique, because poorly chosen iterative solution procedures often require a limit on the time-step size for proper convergence of the iteration.

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